United States
Environmental Protection
Agency

Environmental
Research Laboratory
Athens, GA 30605-2700

Research and Development

EPA/600/SR-95/039 March 1995

EPA

Project Summary

Environmental Fate Constants for Additional 27 Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects

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Under Section 301 of the Resource Conservation and Recovery Act, The U.S. Environmental Protection Agency's (EPA's) Office of Solid Waste is in the process of identifying chemicals to be considered in projects called the hazardous waste identification projects. At this time, there are more than 200 chemical constituents identified in these projects. A previous publication (EPA/600/R-93/132) addressed environmental fate constants and chemical hydrolysis pathways for 189 organic chemicals. This publication addresses an additional 27 organic chemicals. Chemical hydrolysis is addressed. Sorption coefficients are presented. The ionization constant is given when this process affects sorption in the environmental pH range. Additionally, values for water solubility, Henry's law constant, vapor pressure, and diffusivity are reported.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report (see Project Report ordering information at back).

Synopsis of Report

Each chemical is structurally presented and the potential for chemical hydrolysis is addressed. Computed values for water solubility, octanol/water partition coefficient, organic-carbon-normalized sediment/water partition coefficient, Henry's law constant, vapor pressure, and diffusivity are given at 25°C. A short definition is given for each parameter. The organic-carbon-normalized sediment/water partition coefficient is given with consideration of ionization if this process occurs within the environmental pH range.

Table 1. *Data for Physical and Chemical Process Parameters*

	Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K_{oc}	Sorption Log_{ow}	Henry's Law Constant (atm-m^3/mol)	Vapor Pressure (torr)	Diffusivity in Air (cm^2/s)	Hydrolysis
1.	*Anthracene*	120-12-7	7.6E-2	4.21	4.53	1.9E-5	6.1E-6	0.055	NHFG
2.	*Benzenethiol*[a] pk_a = 6.5	108-98-5	7.6E2	1.32	2.35	4.4E-4	2.4	0.076	NLFG oxidizes
3.	*Benzo*[g,h,i]*perylene*	191-24-2	1.2E-4	6.28	6.60	1.2E-7	4.0E-11	0.039	NHFG
4.	*Benzo*[k]*fluoranthene*	207-08-9	9.4E-4	6.0	6.3	5.0E-7	1.4E-9	0.041	NHFG
5.	*Bromobenzene*	108-86-1	4.1E2	2.43	2.75	2.1E-3	4.2	0.073	NLFG[b]
6.	n-*Butylbenzene*	104-51-8	21	3.8	4.1	9.7E-3	1.1	0.060	NHFG
7.	sec-*Butylbenzene*	135-98-8	38	3.6	3.9	9.8E-3	2.1	0.061	NHFG
8.	*Carbazole*	86-74-8	4.0E-1	3.3	3.6	8.6E-7	1.6E-6	0.062	NHFG
9.	*Crotonaldehyde*	4170-30-3	1.3E5	-0.06	0.26	3.1E-5	4.5E1	0.093	
10.	*Dibenzofuran*	132-64-9	4.3	3.8	4.1	1.4E-4	2.7E-3	0.059	NHFG
11.	*1,2,3,4,6,7,8-Heptachlorodibenzofuran*	67562-39-4	9.5E-7	8.20	8.52	3.7E-5	6.5E-11	0.043	NLFG
12.	*1,2,3,4,7,8,9-Heptachlorodibenzofuran*	55673-89-7	1.3E-6	8.2	8.5	3.8E-5	9.5E-11	0.043	NLFG
13.	*1,2,3,4,6,7,8-Heptachlorodibenzo*-p-*dioxin*	35822-46-9	1.9E-7	8.53	8.85	4.1E-5	1.4E-11	0.043	NLFG
14.	*1,2,3,4,7,8-Hexachlorodibenzofuran*	70648-26-9	7.3E-6	7.54	7.86	4.2E-5	6.3E-10	0.045	NLFG
15.	*1,2,3,6,7,8-Hexachlorodibenzofuran*	57117-44-9	6.9E-6	7.55	7.87	4.2E-5	5.9E-10	0.045	NLFG
16.	*1,2,3,7,8,9-Hexachlorodibenzofuran*	72918-21-9	7.3E-6	7.55	7.87	4.3E-5	6.4E-10	0.045	NLFG
17.	*2,3,4,6,7,8-Hexachlorodibenzofuran*	60851-34-5	7.6E-6	7.54	7.86	4.1E-5	6.3E-10	0.045	NLFG
18.	*2-Hexanone*	591-78-6	1.8E4	1.0	1.3	8.7E-5	1.2E1	0.072	NHFG
19.	*Indene*	95-13-6	3.9E2	2.5	2.8	5.0E-4	1.3	0.071	NHFG
20.	p-*Isopropyltoluene*	99-87-6	28	3.7	4.0	9.3E-3	1.5	0.060	NHFG
21.	*2-Methylchrysene*	3351-32-4	8.5E-4	5.82	6.14	1.2E-6	3.1E-9	0.044	NHFG
22.	*1-Methylnaphthalene*	90-12-0	40	3.52	3.84	2.8E-4	6.6E-2	0.060	NHFG
23.	*3-Methylnaphthalene*	91-57-6	33	3.54	3.86	3.0E-4	5.8E-2	0.061	NHFG

(continued)

Table 1. *(Continued)*

Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K_{oc}	Sorption Log_{ow}	Henry's Law Constant (atm-m^3/mol)	Vapor Pressure (torr)	Diffusivity in Air (cm^2/s)	Hydrolysis
24. Phenanthrene	*85-01-8*	*1.1*	*4.25*	*4.57*	*2.3E-5*	*1.0E-4*	*0.055*	*NHFG*
25. n-*Propylbenzene*	*103-65-1*	*57*	*3.35*	*3.67*	*9.9E-3*	*3.6*	*0.065*	*NHFG*
26. 1,2,4-Trimethylbenzene	*95-63-6*	*70*	*3.28*	*3.60*	*4.9E-3*	*2.2*	*0.065*	*NHFG*
27. 1,3,5-Trimethylbenzene	*108-67-8*	*67*	*3.37*	*3.69*	*6.3E-3*	*2.7*	*0.065*	*NHFG*

a. Values reported are for neutral species.
b. Bromobenzene was tested in the laboratory for hydrolysis. No disappearance was noted after 29 days at 85°C in 0.1N sodium hydroxide and 0.1N hydrochloric acid.

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The complete report, entitled "Environmental Fate Constants for Additional 27 Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects," (Order No. PB95-188074; Cost: $17.50, subject to change) will be available only from

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